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PASSWORD:

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NEWS Web Page URLs for STN Seminar Schedule - N. America BLAST(R) searching in REGISTRY available in STN on the Web NEWS Jan 25 FSTA has been reloaded and moves to weekly updates Jan 29 NEWS 3 NEWS 4 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency Access via Tymnet and SprintNet Eliminated Effective 3/31/02 NEWS 5 Feb 19 NEWS 6 Mar 08 Gene Names now available in BIOSIS NEWS 7 Mar 22 TOXLIT no longer available NEWS 8 Mar 22 TRCTHERMO no longer available NEWS 9 Mar 28 US Provisional Priorities searched with P in CA/CAplus and USPATFULL NEWS 10 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY NEWS 11 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead. NEWS 12 Apr 08 "Ask CAS" for self-help around the clock NEWS 13 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area

Welcome to STN International

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NEWS 14 Apr 09 ZDB will be removed from STN
NEWS 15 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 16 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 17 Apr 22 BIOSIS Gene Names now available in TOXCENTER
NEWS 18 Apr 22 Federal Research in Progress (FEDRIP) now available

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002

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NEWS INTER General Internet Information
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN NEWS WWW CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 14:21:56 ON 15 MAY 2002

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 0.21 0.21

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STRUCTURE FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0 DICTIONARY FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

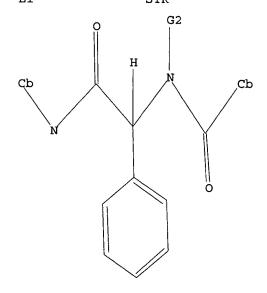
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 09852965-3.str

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 G2 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

09/852,965

SAMPLE SEARCH INITIATED 14:22:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1673 TO ITERATE

59.8% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 31007 TO 35913 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss ful FULL SEARCH INITIATED 14:22:53 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 32586 TO ITERATE

100.0% PROCESSED 32586 ITERATIONS 27 ANSWERS SEARCH TIME: 00.00.04

L3 27 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
140.66
140.87

FILE 'CAPLUS' ENTERED AT 14:23:04 ON 15 MAY 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 15 May 2002 VOL 136 ISS 20 FILE LAST UPDATED: 13 May 2002 (20020513/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 13 L4 13 L3

=> d 14 1-13 bib hitstr

```
ANSWER 1 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
AN
       2001:453049 CAPLUS
DN
       135:45999
       Synthesis and use of serine protease inhibitors (substituted phenylglycine
ΤI
       derivatives) as antiinflammatory agents
       Lively, Sarah Elizabeth; Waszkowycz, Bohdan; Harrison, Martin James;
IN
       Farthing, Christopher Neil; Johnson, Keith Michael
       Protherics Molecular Design Limited, UK
PA
       PCT Int. Appl., 171 pp.
so
       CODEN: PIXXD2
DT
       Patent
       English
LA
FAN.CNT 11
                                                           APPLICATION NO. DATE
       PATENT NO.
                              KIND DATE
                                                            _____
                              _ _ _ _
                                       20010621
                                                           WO 2000-GB4764
                                                                                 20001213
       WO 2001044226
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                  BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                          WO 2000-GB2291 20000613
       WO 2000077027
                               A2
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       WO 2000077027
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                                                          WO 2001-GB2566 20010612
       WO 2001096305
                               A1
                                      20011220
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PRAI GB 1999-29552
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                                       19991214
       WO 2000-GB2291
                                W
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       GB 1999-13823
                                Α
                                       19990614
       US 1999-142064P
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                                       19990702
       GB 1999-18741
                                Α
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       GB 1999-29553
                                Α
                                       19991214
       WO 2000-GB4764
                                W
                                       20001213
os
       MARPAT 135:45999
IT
       344933-13-7P 344933-14-8P 344933-15-9P
       RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
           (synthesis and use of (hetero) arom. substituted phenylglycine derivs.
           as antiinflammatory agents)
RN
       344933-13-7 CAPLUS
```

CN Carbamic acid, [[3-[[2-[(2,3-dihydro-1H-inden-5-yl)amino]-1-(4methylphenyl) -2-oxoethyl] [(2,4-dimethoxyphenyl) methyl] amino] carbonyl] pheny 1]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN

344933-14-8 CAPLUS Benzoic acid, 4-[2-[(2,3-dihydro-1H-inden-5-yl)amino]-1-[[(2,4-CN dimethoxyphenyl) methyl] [3-[[[(1,1-dimethylethoxy) carbonyl] amino] methyl] ben
zoyl] amino] -2-oxoethyl] -, methyl ester (9CI) (CA INDEX NAME)

RN

344933-15-9 CAPLUS
Benzoic acid, 4-[2-[(2,3-dihydro-1H-inden-5-yl)amino]-1-[[(2,4-CN dimethoxyphenyl) methyl] [3-[[[(1,1-dimethylethoxy)carbonyl]amino]methyl]ben zoyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
       2001:167962 CAPLUS
AN
       134:222529
DN
       Preparation of aromatic trifluoromethylsulfonyl and
TI
       trifluoromethylsulfonamido compounds as phosphate mimics and phosphatase
       inhibitors and methods of treatment
       Huang, Ping; Wei, Chung Chen; Tang, Peng Cho; Liang, Chris; Ramphal, John;
IN
       Jallal, Bahija; Blitz, John; Li, Sharon; Mattson, Matthew Neil; Mcahon,
       Gerald; Koenig, Marcel
PΑ
       Sugen, Inc., USA; et al.
       PCT Int. Appl., 262 pp.
SO
       CODEN: PIXXD2
DT
       Patent
      English
LA
FAN.CNT 1
       PATENT NO.
                              KIND DATE
                                                            APPLICATION NO. DATE
                               A1 20010308 🗶
                                                            WO 2000-US23293 20000825
PΙ
       WO 2001016097
            W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                       19990827
PRAI US 1999-150970P
                              P
       US 1999-165365P
                                Р
                                       19991112
os
       MARPAT 134:222529
       329317-75-1P, N-Cyclohexyl-N-[(2,6-dimethylphenylcarbamoyl)-(4-
       trifluoromethanesulfonylphenyl) methyl]benzamide
       RL: BAC (Biological activity or effector, except adverse); BSU (Biological
       study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
       BIOL (Biological study); PREP (Preparation); USES (Uses)
           (drug candidate; prepn. of arom. trifluoromethylsulfonyl and
           trifluoromethylsulfonamido compds. as phosphate mimics and phosphatase
           inhibitors)
```

329317-75-1 CAPLUS RN

Benzeneacetamide, .alpha.-(benzoylcyclohexylamino)-N-(2,6-dimethylphenyl)-CN4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 13 CAPLUS COPYRIGHT 2002 ACS L4

2001:50635 CAPLUS AN

DN 134:115845

Preparation of .alpha.,.beta.-annelated butyrolactones as modulators of ΤI metabotropic glutamate receptors.

Stolle, Andreas; Antonicek, Horst-Peter; Lensky, Stephan; Voerste, Arnd; IN Muller, Thomas; Baumgarten, Jorg; Von Dem Bruch, Karsten; Muller, Gerhard; Stropp, Udo; Horvath, Ervin; De Vry, Jean-Marie-Victor; Schreiber, Rudy

PABayer Aktiengesellschaft, Germany

SO PCT Int. Appl., 215 pp.

CODEN: PIXXD2

Patent DT

LA German

FAN.CNT 1

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PATENT NO.
                                             KIND
                                                         DATE
                                                                                         APPLICATION NO. DATE
                                             _ _ _ _
                                                          _____
                                                                                         _____
          WO 2001004107
                                              A1
                                                          20010118
                                                                                         WO 2000-EP6105
                                                                                                                            20000630
PΙ
                 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
                  RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                                                       DE 1999-19932621 19990713
          DE 19932621
                                               A1
                                                          20010426
PRAI DE 1999-19932621 A
                                                          19990713
          MARPAT 134:115845
IT
          321128-05-6P
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OS

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of .alpha.,.beta.-annelated butyrolactones as modulators of metabotropic glutamate receptors)

RN321128-05-6 CAPLUS

CN Benzeneacetamide, .alpha.-(benzoylmethylamino)-N-[4-[[(3aR,6aR)-tetrahydro-5-methylene-3-oxo-1H-cyclopenta[c]furan-3a(3H)-yl]methyl]phenyl]-, rel-

(9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 2000:454829 CAPLUS

DN 133:222996

TI Multicomponent synthesis of novel amino acid-nucleobase chimeras: a versatile approach to PNA-monomers

AU Maison, Wolfgang; Schlemminger, Imre; Westerhoff, Ole; Martens, Jurgen

CS Fachbereich Chemie, Universitat Oldenburg, Oldenburg, D-26111, Germany

SO Bioorganic & Medicinal Chemistry (2000), 8(6), 1343-1360 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 133:222996

IT 292072-91-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(multicomponent synthesis of novel amino acid-nucleobase chimeras for use as PNA-monomers)

RN 292072-91-4 CAPLUS

CN Carbamic acid, [1-[[2-[[[2-(acetylamino)ethyl] [2-[[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl]amino]-2-oxo-1-phenylethyl]amino]carbonyl]phenyl]methyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 70 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 13 CAPLUS COPYRIGHT 2002 ACS L4

2000:53602 CAPLUS AN

132:108299 DN

Preparation of precursors for PNA monomers TТ

Martens, Jurgen; Maison, Wolfgang; Schlemminger, Imre; Westerhoff, Ole; IN Groger, Harald

PA Germany

PCT Int. Appl., 72 pp. SO CODEN: PIXXD2

DTPatent

English LA

FAN.CNT 1

APPLICATION NO. DATE PATENT NO. KIND DATE ______ _ _ _ _ 19980710 WO 1998-EP4281 PΙ WO 2000002864 A1 20000120 W: AT, AU, BG, BR, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HR, HU, IL, JP, KR, LU, MK, MX, NO, NZ, PL, PT, RU, SE, SI, TR, US, YU
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG AU 1998-90645 AU 9890645 A1 20000201 19980710 19980710

PRAI WO 1998-EP4281 Α

os MARPAT 132:108299

IT 255736-69-7P 255736-75-5P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of precursors for PNA monomers)

RN255736-69-7 CAPLUS

Carbamic acid, [2-[[2-(1-cyclohexen-1-ylamino)-2-oxo-1-phenylethyl] [2-CN [(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)methyl]benzoyl]amino]et hyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

255736-75-5 CAPLUS RN

Benzeneacetamide, .alpha.-[[2-[(3,4-dihydro-2,4-dioxo-1(2H)-CN pyrimidinyl) methyl] benzoyl] [2-[(2-methyl-1-oxopropyl) amino] phenyl] amino] -N-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl]- (9CI) (CA INDEX NAME)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2002 ACS
- AN 1999:662324 CAPLUS
- DN 132:64501
- TI Generation of an Ugi library of phosphate mimic-containing compounds and identification of novel dual specific phosphatase inhibitors
- AU Bergnes, Gustave; Gilliam, Carla L.; Boisclair, Michael D.; Blanchard, Jill L.; Blake, Katharine V.; Epstein, David M.; Pal, Kollol
- CS Department of Medicinal Chemistry, Mitotix, Inc., Cambridge, MA, 02139,
- SO Bioorganic & Medicinal Chemistry Letters (1999), 9(19), 2849-2854 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- IT 253132-59-1P 253132-61-5P 253132-62-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(using the combinatorial Ugi reaction to prep. a library of dipeptidyl phosphate mimics to identify the binding requirements of Cdc25 phosphatase)

- RN 253132-59-1 CAPLUS
- CN Propanedioic acid, [4-[[(1,3-benzodioxol-5-ylmethyl) [2-(cyclohexylamino)-2oxo-1-[4-(phosphonomethoxy)phenyl]ethyl]amino]carbonyl]phenoxy]- (9CI)
 (CA INDEX NAME)

RN 253132-61-5 CAPLUS

CN Propanedioic acid, [4-[1-[(1,3-benzodioxol-5-ylmethyl)] [4-(phosphonomethyl)benzoyl]amino]-2-(cyclohexylamino)-2-oxoethyl]phenoxy]-(9CI) (CA INDEX NAME)

RN 253132-62-6 CAPLUS

CN Propanedioic acid, [4-[[(1,3-benzodioxol-5-ylmethyl) [2-(cyclohexylamino)-1-[4-(dicarboxymethoxy)phenyl]-2-oxoethyl]amino]carbonyl]phenoxy]- (9CI) (CA INDEX NAME)

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 1999:45211 CAPLUS

DN 130:110408

TI Preparation of fluorous silicon, tin and germanium compounds and their use in organic synthesis to facilitate organic/fluorous extractive purification

IN Curran, Dennis P.; Hadida, Ruah Sabine; Hoshino, Masahide; Studer, Armido; Wipf, Peter; Jeger, Patrick; Kim, Sun-young; Ferritto, Rafael

PA University of Pittsburgh, USA

SO U.S., 40 pp., Cont.-in-part of U.S. 5,777,121. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

PAN. CNI Z																			
	PATENT NO.				KIND		DATE			/ A	PPLI	CATI	ON NO	Э.	DATE				
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ΡI	US	5859247			A		19990112			U	3 1996-690491				19960731				
	US	5777121			A		19980707			US 1996-67194			7194	5	19960628				
	CA	2259183			AA		19980108			C	CA 1997-2259183 1997062								
	WO	9800	376		Α	19980108				WO 1997-US11215						19970626			
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			GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	
			GN,	ML,	MR,	ΝE,	SN,	TD,	TG										
	ΑU	AU 9735818			A1 19980121					AU 1997-35818					19970626				
	EP	9076	25		Α	1	19990414			EP 1997-932333				3	19970626				
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	JP	2000	5140	62	T2		20001024			JP 1998-504319 19970626									

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US 6156896
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PRAI US 1996-671945
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    US 1996-690491
                      Α
                            19960731
                      W
    WO 1997-US11215
                            19970626
    CASREACT 130:110408; MARPAT 130:110408
O.S
    189077-35-8P
IT
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. from fluorous silylbenzoic acid, amine, aldehyde and isocyanide
       using org./fluorous extractive purifn.)
     189077-35-8 CAPLUS
RN
    Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-cyclohexyl- (9CI)
CN
       (CA INDEX NAME)
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RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

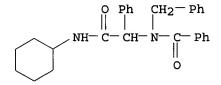
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ANSWER 8 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
AN
      1998:55597 CAPLUS
DN
      128:127604
      Fluorous reaction and separation systems
TΙ
      Curran, Dennis P.; Hadida, Ruah Sabine; Hashino, Masahide; Studer, Armido;
IN
      Wipf, Peter; Jeger, Patrick; Kim, Sun-young; Ferritto, Rafael
PA
      University of Pittsburgh, USA
      PCT Int. Appl., 120 pp.
SO
      CODEN: PIXXD2
DT
      Patent
      English
LΑ
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      PATENT NO.
                             KIND DATE
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                                                          WO 1997-US11215 19970626
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      WO 9800376
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                               W
                                      19970626
OS
      CASREACT 128:127604; MARPAT 128:127604
IT
      189077-35-8P
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RL: SPN (Synthetic preparation); PREP (Preparation)
 (fluorous reaction and sepn. systems)

RN 189077-35-8 CAPLUS

CN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-cyclohexyl- (9CI) (CA INDEX NAME)





- L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2002 ACS
- AN 1997:253978 CAPLUS
- DN 126:292891
- TI Fluorous Synthesis: Fluorous Protocols for the Ugi and Biginelli Multicomponent Condensations

AU Studer, Armido; Jeger, Patrick; Wipf, Peter; Curran, Dennis P.

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO J. Org. Chem. (1997), 62(9), 2917-2924 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

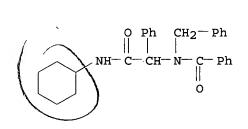
OS CASREACT 126:292891

IT 189077-35-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (application of fluorous protocols for Ugi and Biginelli multicomponent condensations)

RN 189077-35-8 CAPLUS

CN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-cyclohexyl- (9CI) (CA INDEX NAME)





- L4 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2002 ACS
- AN 1996:133173 CAPLUS
- DN 124:289157
- TI Postcondensation Modifications of Ugi Four-Component Condensation Products: 1-Isocyanocyclohexene as a Convertible Isocyanide. Mechanism of Conversion, Synthesis of Diverse Structures, and Demonstration of Resin Capture

AU Keating, Thomas A.; Armstrong, Robert W.

CS Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, 90095, USA

SO J. Am. Chem. Soc. (1996), 118(11), 2574-83 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

IT 175606-32-3

RL: RCT (Reactant)

(modified of Ugi four-component condensation by use of isocyanatocyclohexene as isocyanide equiv.)

RN 175606-32-3 CAPLUS

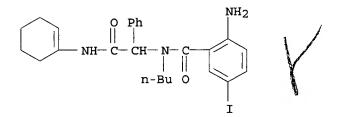
CN Benzeneacetamide, .alpha.-(benzoylbutylamino)-N-1-cyclohexen-1-yl- (9CI) (CA INDEX NAME)

IT 175606-23-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (modified of Ugi four-component condensation by use of isocyanocyclohexene as isocyanide equiv.)

RN 175606-23-2 CAPLUS

CN Benzeneacetamide, .alpha.-[(2-amino-5-iodobenzoyl)butylamino]-N-1-cyclohexen-1-yl- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 1989:422724 CAPLUS

DN 111:22724

TI Organic syntheses via transition metal complexes. 35.
(C-Amino)keteneimines, 2-imidazolin-5-ones, and .alpha.-amino acids from aminocarbene chromium complexes and isocyanides

AU Aumann, Rudolf; Heinen, Heinrich

CS Org. Chem. Inst., Univ. Muenster, Muenster, D-4400, Fed. Rep. Ger.

SO Chem. Ber. (1989), 122(6), 1139-45 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 111:22724

IT 119209-05-1P

RN 119209-05-1 CAPLUS

CN Benzeneacetamide, N-cyclohexyl-.alpha.-(dibenzoylamino)- (9CI) (CA INDEX NAME)

```
ANSWER 12 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
    1970:477105 CAPLUS
AN
DN
     73:77105
     Preparation and properties of mesoionic oxazolones
ΤI
     Bayer, Horst O.; Huisgen, Rolf; Knorr, Rudolf; Schaefer, Fred C.
ΑU
     Inst. Org. Chem., Univ. Muenchen, Munich, Ger.
CS
so
     Chem. Ber. (1970), 103(8), 2581-97
     CODEN: CHBEAM
DT
     Journal
     German
LA
     28544-59-4P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     28544-59-4 CAPLUS
     Benzamide, N-methyl-N-[.alpha.-(p-tolylcarbamoyl)benzyl]- (8CI) (CA INDEX
CN
     NAME)
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ANSWER 13 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
AN
     1967:2461 CAPLUS
     66:2461
DN
     2,3,4,5-Tetrahydro-1H-3-benzazepin-1-ones and
ΤI
     hexahydroimidazoisoquinolines
ΑU
     Hazebroucq, Georges
     Pharm., Centrale Hop., Paris, Fr.
CS
     Ann. Chim. (Paris) (1966), 1(5/6), 221-54
SO
     CODEN: ANCPAC
DT
     Journal
     French
LΑ
IT
     14174-20-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     14174-20-0 CAPLUS
     Acetanilide, 2-[N-(3,4-dimethoxyphenethyl)benzamido]-2-phenyl- (8CI)
CN
     INDEX NAME)
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=> log y COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 40.12 180.99

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 14:23:35 ON 15 MAY 2002

Welcome to STN International! Enter x:x

LOGINID:ssspta1611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 11 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead.
NEWS 12 Apr 08 "Ask CAS" for self-help around the clock
NEWS 13 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 14 Apr 09 ZDB will be removed from STN
NEWS 15 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 16 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS NEWS 17 Apr 22 BIOSIS Gene Names now available in TOXCENTER NEWS 18 Apr 22 Federal Research in Progress (FEDRIP) now available NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002 NEWS HOURS STN Operating Hours Plus Help Desk Availability

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CAS World Wide Web Site (general information)

FILE 'HOME' ENTERED AT 14:02:57 ON 15 MAY 2002

=> ile reg
ILE IS NOT A RECOGNIZED COMMAND

09/810,648

NEWS INTER

NEWS LOGIN

NEWS PHONE

NEWS WWW

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:03:07 ON 15 MAY 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0 DICTIONARY FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

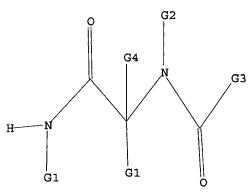
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb,Ak

G4 H,Me

Structure attributes must be viewed using STN Express query preparation.

09/810,648

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2.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

45 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
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PROJECTED ITERATIONS: 815485 TO 839635 PROJECTED ANSWERS: 34653 TO 39827

L2 45 SEA SSS SAM L1

=> d scan

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-Nmethylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanyl-D-alanylN-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N,N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]- (9CI)

SQL 11 MF C79 H125 N11 O17

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):44

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2 (1H) -Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4-dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C29 H34 N4 O4 S

$$\begin{array}{c|c} & & & & \\ & & & \\ & & \\ H_2N & & C-CH_2 \\ \hline & & N-C-CH_2-CH_2-N \\ \hline & & \\ & & \\ O \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

$$\begin{array}{c|c} & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ &$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl-, [S-(R*,R*)]- (9CI)
C34 H58 N4 O7 IN

MF

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-1-oxo-Npropyl-3-(2-quinolinyl)-7-[(2,3,5,6-tetrafluoro-4-methylbenzoyl)amino](9CI)

MF C34 H31 F4 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide
, 45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-

3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)
MF C88 H115 N33 O32

PAGE 1-A

Me NH

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 $C=0$
 $N-CH_2-C-NH_2$
 CH_2
 CH_2
 NH
 CH_2
 NH
 CH_2
 CH_2

PAGE 1-B

PAGE 1-C

PAGE 2-C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-D-isoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL 10

MF C49 H85 N15 O15

Absolute stereochemistry.

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)

MF C35 H42 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Dermorphin, 2-D-arginine-4-(N-methylglycine) - (9CI)

SQL 7

MF C44 H59 N11 O10

PAGE 1-B

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . Cl H

HCl

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)(2-methoxyethyl)amino]carbonyl]phenyl]methyl]-N-[(2-chlorophenyl)methyl]1,2,3,4-tetrahydro-3-(2-methoxyphenyl)-1-oxo-(9CI)

MF C37 H37 C1 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Glycine, 2-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-N-methyl-3(methylsulfonyl)-L-alanyl-3-amino-2-hydroxyhexanoylglycyl-2-phenyl-,
1,1-dimethylethyl ester, (2S)- (9CI)

SQL 5
MF C38 H61 N5 Oll S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN D-Alaninamide, N-[(tetrahydro-2-furanyl)carbonyl]glycyl-3-(2-naphthalenyl) D-alanyl-4-chloro-D-phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-N-methyl L-tyrosyl-N6-(3-pyridinylcarbonyl)-L-lysyl-L-leucyl-N6-(1-methylethyl)-L lysyl-L-prolyl-, (S)- (9CI)
SQL 11
MF C85 H111 Cl N16 O16
CI COM

PAGE 1-A

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI) MF C28 H33 N5 O4

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{N} \\ \text{C} \\ \text$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 7-Oxa-2,5,10,13-tetraazatetradecan-14-oic acid, 10-[2-[[1-(cyclohexylmethyl)-2-hydroxy-5-methylhexyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-2,5-dimethyl-1-(4-morpholinyl)-1,6,9-trioxo-8-(phenylmethyl)-, phenylmethyl ester, [1S-[1R*[R*(R*)],2R*]]- (9CI)

MF C49 H72 N8 O9

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[[2(trimethylsilyl)ethoxy]carbonyl]amino]-D-alanyl-L-alanyl-S[(acetylamino)methyl]-N-methyl-L-cysteinyl-N-methyl-L-valyl-(2R)-2-[[(1,1dimethylethoxy)carbonyl]amino]-.beta.-alanyl-L-alanyl-S[(acetylamino)methyl]-N-methyl-L-cysteinyl-N-methyl-, methyl ester (9CI)
SQL 8
MF C55 H100 N12 O17 S2 Si

PAGE 1-B

PAGE 1-A

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(2-

fluorobenzoyl)amino]-3,4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl)- (9CI)

MF C33 H32 F N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-

valyl]-L-isoleucyl]-L-asparaginyl]-L-.alpha.-aspartyl]- (9CI)
SQL 5
MF C35 H54 N6 O12

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C22 H32 N4 O2 . x C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
methyl ester (9CI)

MF C42 H34 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-Nmethyl-3-(2-naphthalenyl)-D-alanyl-N,N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-O-(1,1-dimethylethyl)-N-methyl-L-tyrosyl-D-alanylglycyl-N-[1-(hydroxymethyl)-3-(methylthio)propyl]-N.alpha.-propyl-, (S)- (9CI)

SQL 5

MF C41 H63 N5 O8 S

PAGE 1-A

CH2-Ph

O Me

| O CH2-OH

| | | |

t-BuO-C-N O Me O O CH-C-NH-CH-CH2
CH2-CH-C-NH-CH-C-NH-CH2-C-N-Pr-n

PAGE 1-B

- CH $_2$ - SMe

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-

methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

PAGE 2-B

PAGE 3-A

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(2-methoxyphenyl)-1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

MF C37 H36 F3 N5 O5

PAGE 1-A

$$\begin{array}{c} \text{CF}_3 \\ \text{CH}_2 \\ \text{NH} \\ \text{CH}_2 - \text{CH}_2 - \text{N} - \text{C} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \text{N} \\ \text{H}_2 \text{N} - \text{C} - \text{CH}_2 \\ \text{O} \end{array}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl[(3-methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
methyl ester (9CI)

MF C44 H55 Cl N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

45 ANSWERS REGISTRY COPYRIGHT 2002 ACS L2

2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[[(2-IN chlorophenyl) methyl] amino] carbonyl] -3, 4-dihydro-3-[4-(methylthio) phenyl] -1oxo-N-(3-pyridinylmethyl) - (9CI) C35 H34 Cl N5 O4 S

MF

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & & \\ & & & \\ H_2N-C-CH_2 & & & \\ & &$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (phenylmethyl) amino] carbonyl] phenyl] methyl] -1,2,3,4-tetrahydro-3-(4-hydroxyphenyl)-1-oxo-N-[[4-(trifluoromethyl) phenyl] methyl] - (9CI)
MF C41 H35 F3 N4 O5

$$\begin{array}{c} \text{CF}_3 \\ \text{CH}_2 \\ \text{NH} \\ \text{O} \\ \text{CH}_2 \\ \text{NH} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{NH} \\ \text{O} \\ \text{O}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L.alpha.-aspartyl]-, mono(trifluoroacetate) (9CI)
SQL 4
MF C20 H31 N5 O7 . C2 H F3 O2
CM 1

$$(CH_2)_4$$
 N
 $(CH_2)_4$
 N
 N
 S
 CO_2H
 CO_2H
 CO_2H
 S
 $Pr-i$

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

MF C37 H51 Cl N4 O7

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)

MF C37 H39 N5 O5 S

PAGE 1-A

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-[(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-(9CI)

MF C33 H33 F2 N5 O5

Eto- (CH₂)₃-N-C-CH₂-CH₂

$$H_2N-C-CH_2$$

O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-D phenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysyl L-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl (9CI)

SQL 13

MF C94 H135 Cl N30 O18

45 ANSWERS L2REGISTRY COPYRIGHT 2002 ACS

Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-IN biphenyl]-4-yl- (9CI) C33 H42 N4 O4

MF

Ph
$$CH_2 - C - NH_2 O \\ N - C - CH_2 - N - C - CH_2 - NH - CH_2 - CH_2 \\ O (CH_2)_5 - Me$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl-4-fluoro- (9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

SINCE FILE ENTRY SESSION

TOTAL

FULL ESTIMATED COST

0.76 0.97

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TERMINAL (ENTER 1, 2, 3, OR ?):2

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COST IN U.S. DOLLARS

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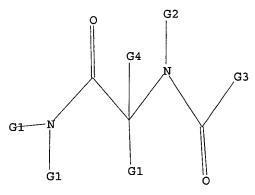
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb,Ak

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam SAMPLE SEARCH INITIATED 13:03:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 41378 TO ITERATE

2.4% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

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PROJECTED ITERATIONS:

815485 TO 839635

PROJECTED ANSWERS:

37850 TO 43250

49 ANSWERS

L2 49 SEA SSS SAM L1

3/850 10 432

=> d scan

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6-methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C28 H33 N5 O4

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{O} \\ \text{O} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):48

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl, [S-(R*,R*)]- (9CI)

MF C34 H58 N4 O7

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2 (1H) -Isoquinolinepropanamide, N-(2-amino-2-oxoethyl) -7-[(2-fluorobenzoyl) amino] -3, 4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl) - (9CI)

MF C33 H32 F N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN .beta.-Alanine, N-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]ph
enyl]acetyl]-N-(3-phenylpropyl)glycyl-N-(3-phenylpropyl)- (9CI)

MF C40 H46 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
methyl ester (9CI)

MF C42 H34 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)(2-methoxyethyl)amino]carbonyl]phenyl]methyl]-N-[(2-chlorophenyl)methyl]1,2,3,4-tetrahydro-3-(2-methoxyphenyl)-1-oxo-(9CI)
- MF C37 H37 Cl N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-Nmethylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanyl-D-alanylN-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N,N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]- (9CI)

SQL 11

MF C79 H125 N11 O17

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-Disoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL 10

MF C49 H85 N15 O15

PAGE 1-A

PAGE 1-B

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS L-Leucine, N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-valyl]-L-isoleucyl]-L-asparaginyl]-L-alpha.-aspartyl]- (9CI) IN

SQL

C35 H54 N6 O12 MF

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

$$\begin{array}{c|cccc} O & Ph & O \\ || & | & || \\ Ph-C-N-CH-C-NHBu-t \\ & & | \\ Ph-CH_2 \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

TN Glycine 2-cyclohexyl-N-[(1 1-dimethylethoxy)ca

SQL 5

MF C38 H61 N5 O11 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-3-(4-methylphenyl)-1-oxo-4-[[(3-pyridinylmethyl)amino]carbonyl]- (9CI)

MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L.alpha.-aspartyl]-, mono(trifluoroacetate) (9CI)
SQL 4
MF C20 H31 N5 O7 . C2 H F3 O2
CM 1

Absolute stereochemistry.

$$(CH_2)_4$$
 $(CH_2)_4$
 $(CH_$

CM 2

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)
MF C35 H42 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl]- (9CI)

MF C38 H40 N4 O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . Cl H

● HCl

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C29 H34 N4 O4 S

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ H_2N & C - CH_2 \\ \hline & & \\ & N - C - CH_2 - CH_2 - N \\ \hline & & \\ & & \\ & & \\ & & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl[(3-methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
 methyl ester (9CI)
MF C44 H55 Cl N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C34 H31 F4 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalanine, N-[(2E)-5-amino-5-methyl-1-oxo-2-hexenyl]-3-[1,1'-biphenyl]-4-yl-N-methyl-D-alanyl-N-methyl-, trimethylhydrazide (9CI)

MF C36 H47 N5 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Dermorphin, 2-D-arginine-4-(N-methylglycine)- (9CI)
SQL 7
MF C44 H59 N11 O10

PAGE 1-B

__OH

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

PAGE 2-B

PAGE 3-A

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl-1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2002 ACS L249 ANSWERS

D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]-IN D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

C37 H51 Cl N4 O7 MF

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[[(3-carboxyphenyl)amino]carbonyl]glycyl-N-methyl-N-phenyl-IN N2-8-quinolinyl- (9CI)

C28 H25 N5 O5 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-[(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-(9CI)

MF C33 H33 F2 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-biphenyl]-4-yl- (9CI)

MF C33 H42 N4 O4

Ph
$$CH_2 - C - NH_2 O \\ N - C - CH_2 - N - C - CH_2 - NH - CH_2 - CH_2 \\ O (CH_2)_5 - Me$$
 OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl4-fluoro- (9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[(2chlorophenyl)methyl]amino]carbonyl]-3,4-dihydro-3-[4-(methylthio)phenyl]-1oxo-N-(3-pyridinylmethyl)- (9CI)

MF C35 H34 Cl N5 O4 S

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ H_2N-C-CH_2 & & \\ & & & \\ N & & CH_2-N-C-CH_2-CH_2-N \\ & & & \\ \end{array}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 7-Oxa-2,5,10,13-tetraazatetradecan-14-oic acid, 10-[2-[[1-

 $\label{lem:cyclohexylmethyl} $$ (cyclohexylmethyl) -2-hydroxy-5-methylhexyl]$ amino] -1-(1H-imidazol-4-ylmethyl) -2-oxoethyl] -2,5-dimethyl-1-(4-morpholinyl) -1,6,9-trioxo-8-(phenylmethyl) -, phenylmethyl ester, [1S-[1R*[R*(R*)],2R*]] - (9CI)$

MF C49 H72 N8 O9

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)
MF C37 H39 N5 O5 S

PAGE 1-A

O CH₂-C-NH₂

O CH₂-C-NH₂

O CH₂-C-NH₂

O CH₂-CH₂-CH₂

SMe

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-D phenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysyl L-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl (9CI)

SQL 13

MF C94 H135 Cl N30 O18

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

NH2

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(2-methoxyphenyl)-1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

MF C37 H36 F3 N5 O5

PAGE 1-A

PAGE 1-B

$$\begin{array}{c} \text{CF}_3 \\ \text{CH}_2 \\ \text{NH} \\ \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{N} - \text{C} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \text{N} \\ \text{H}_2 \text{N} - \text{C} - \text{CH}_2 \\ \text{O} \end{array}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-[(tetrahydro-2-furanyl)carbonyl]glycyl-3-(2-naphthalenyl)D-alanyl-4-chloro-D-phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-N-methylL-tyrosyl-N6-(3-pyridinylcarbonyl)-L-lysyl-L-leucyl-N6-(1-methylethyl)-Llysyl-L-prolyl-, (S)- (9CI)

SQL 11

MF C85 H111 Cl N16 O16

CI COM

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (phenylmethyl) amino] carbonyl] phenyl] methyl] -1,2,3,4-tetrahydro-3-(4-hydroxyphenyl) -1-oxo-N-[[4-(trifluoromethyl) phenyl] methyl] - (9CI)
MF C41 H35 F3 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Ornithinamide, L-leucyl-N2-methyl-N-2-naphthalenyl-, trifluoroacetate (9CI)

MF C22 H32 N4 O2 . x C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Glycinamide, N-[[(3-methylphenyl)amino]carbonyl]glycyl-N-methyl-N2-[3-[2oxo-2-(phenylamino)ethoxy]phenyl]-N-phenyl- (9CI)

MF C33 H33 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl
ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C55 H100 N12 O17 S2 Si

PAGE 1-A

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide
, 45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)

MF C88 H115 N33 O32

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-C

$$-NH-C-CH_2-N-C-CH_2-N$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-N-methyl-3-(2-naphthalenyl)-D-alanyl-N,N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-O-(1,1dimethylethyl)-N-methyl-L-tyrosyl-D-alanylglycyl-N-[1-(hydroxymethyl)-3(methylthio)propyl]-N.alpha.-propyl-, (S)- (9CI)

SQL 5

MF C41 H63 N5 O8 S

PAGE 1-A

PAGE 1-B

— CH2- SMe

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.76 0.97

STN INTERNATIONAL LOGOFF AT 13:04:40 ON 15 MAY 2002

Welcome to STN International! Enter x:x

LOGINID:ssspta1611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

Welcome to STN International * * * * * * * * * Web Page URLs for STN Seminar Schedule - N. America NEWS BLAST(R) searching in REGISTRY available in STN on the Web 2 Jan 25 NEWS FSTA has been reloaded and moves to weekly updates NEWS DKILIT now produced by FIZ Karlsruhe and has a new update NEWS 4 Feb 01 frequency Access via Tymnet and SprintNet Eliminated Effective 3/31/02 NEWS 5 Feb 19 Gene Names now available in BIOSIS NEWS 6 Mar 08 NEWS 7 Mar 22 NEWS 8 Mar 22 TOXLIT no longer available TRCTHERMO no longer available NEWS 9 Mar 28 US Provisional Priorities searched with P in CA/CAplus and USPATFULL NEWS 10 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY NEWS 11 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead. NEWS 12 Apr 08 "Ask CAS" for self-help around the clock NEWS 13 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area NEWS 14 Apr 09 ZDB will be removed from STN
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CAS World Wide Web Site (general information)

FILE 'HOME' ENTERED AT 14:02:57 ON 15 MAY 2002

=> ile reg
ILE IS NOT A RECOGNIZED COMMAND

09/852,965

NEWS WWW

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21

0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:03:07 ON 15 MAY 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0 DICTIONARY FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

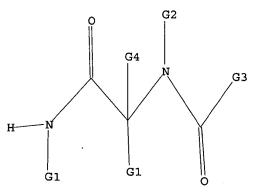
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

Uploading 09852965-2.str

STRUCTURE UPLOADED L1

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb, Ak

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

09/852,965

=> s l1 sss sam SAMPLE SEARCH INITIATED 14:03:36 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 41378 TO ITERATE

2.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 45 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 815485 TO 839635

L2 45 SEA SSS SAM L1

=> d scan

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-Nmethylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanyl-D-alanylN-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N,N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]- (9CI)

39827

34653 TO

SQL 11 MF C79 H125 N11 O17

PROJECTED ANSWERS:

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):44

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C29 H34 N4 O4 S

$$\begin{array}{c|c} & & & & \\ & & & \\ & & \\ H_2N & & C - CH_2 \\ & & & \\ & & N - C - CH_2 - CH_2 - N \\ & & & \\ & & & \\ & & & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl, [S-(R*,R*)]- (9CI)

MF C34 H58 N4 O7

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2 (dimethylamino)ethyl]-3,4-dihydro-3-(4-methylphenyl)-1-oxo-4-[[(3-pyridinylmethyl)amino]carbonyl]- (9CI)
- MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-1-oxo-Npropyl-3-(2-quinolinyl)-7-[(2,3,5,6-tetrafluoro-4-methylbenzoyl)amino](9CI)
- MF C34 H31 F4 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide
 , 45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-

MF

3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)
C88 H115 N33 O32

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-C

PAGE 1-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-D-isoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL 10

MF C49 H85 N15 O15

Absolute stereochemistry.

NH₂

NH

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)

MF C35 H42 N6 O4

$$\begin{array}{c} O \\ O \\ CH_2-C-NH_2 \\ O \\ C-N-(CH_2)_3-NEt_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Dermorphin, 2-D-arginine-4-(N-methylglycine)- (9CI)

SQL 7

MF C44 H59 N11 O10

PAGE 1-B

__OH

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI)
MF C38 H40 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . Cl H

● HCl

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (2-methoxyethyl) amino] carbonyl]phenyl]methyl]-N-[(2-chlorophenyl)methyl]1,2,3,4-tetrahydro-3-(2-methoxyphenyl)-1-oxo- (9CI)

MF C37 H37 Cl N4 O6

$$\begin{array}{c} \text{Cl} \\ \text{CH2} \\ \text{NH} \\ \text{OMe} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 5

MF C38 H61 N5 O11 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-[(tetrahydro-2-furanyl)carbonyl]glycyl-3-(2-naphthalenyl)D-alanyl-4-chloro-D-phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-N-methylL-tyrosyl-N6-(3-pyridinylcarbonyl)-L-lysyl-L-leucyl-N6-(1-methylethyl)-Llysyl-L-prolyl-, (S)- (9CI)

SQL 11

MF C85 H111 Cl N16 O16

CI COM

PAGE 1-A

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6-methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C28 H33 N5 O4

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

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- L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C55 H100 N12 O17 S2 Si

PAGE 1-A

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(2-fluorobenzoyl)amino]-3,4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl)- (9CI)

MF C33 H32 F N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-

09/852,965

valyl]-L-isoleucyl]-L-asparaginyl]-L-.alpha.-aspartyl]- (9CI)
SQL 5
MF C35 H54 N6 O12

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C22 H32 N4 O2 . \times C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
methyl ester (9CI)

MF C42 H34 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-N-methyl-3-(2-naphthalenyl)-D-alanyl-N,N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-O-(1,1dimethylethyl)-N-methyl-L-tyrosyl-D-alanylglycyl-N-[1-(hydroxymethyl)-3(methylthio)propyl]-N.alpha.-propyl-, (S)- (9CI)

SQL 5

MF C41 H63 N5 O8 S

PAGE 1-B

- CH2- SMe

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

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PAGE 3-A

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(2-methoxyphenyl)-1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

MF C37 H36 F3 N5 O5

PAGE 1-A

$$\begin{array}{c} \text{CF}_{3} \\ \text{CH}_{2} \\ \text{NH} \\ \text{C} \\ \text{C} \\ \text{O} \\ \text{N} \\ \text{H}_{2}\text{N} - \text{C} - \text{CH}_{2} - \text{CH}_{2} - \text{CH}_{2} \\ \text{O} \\ \end{array}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl](3methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
methyl ester (9CI)

MF C44 H55 Cl N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[[(2-chlorophenyl)methyl]amino]carbonyl]-3,4-dihydro-3-[4-(methylthio)phenyl]-1-oxo-N-(3-pyridinylmethyl)- (9CI)

MF C35 H34 Cl N5 O4 S

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PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

45 ANSWERS REGISTRY COPYRIGHT 2002 ACS L2 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-IN oxoethyl) (phenylmethyl) amino] carbonyl] phenyl] methyl] -1,2,3,4-tetrahydro-3-(4-hydroxyphenyl)-1-oxo-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) C41 H35 F3 N4 O5 MF

$$\begin{array}{c} CF_3 \\ CH_2 \\ NH \\ CH_2 \\ NH \\ CH_2 \\ CH_2 \\ CH_2 \\ NH \\ CH$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

45 ANSWERS REGISTRY COPYRIGHT 2002 ACS L2 L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L-IN .alpha.-aspartyl]-, mono(trifluoroacetate) (9CI) SQL MF C20 H31 N5 O7 . C2 H F3 O2 CM

Absolute stereochemistry.

1

$$(CH_2)_4$$
 Me
 O
 H
 CO_2H
 CO_2

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

MF C37 H51 Cl N4 O7

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)

MF C37 H39 N5 O5 S

PAGE 1-A

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-[(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-(9CI)

MF C33 H33 F2 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-Dphenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysylL-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl(9CI)

SQL 13

MF C94 H135 Cl N30 O18

REGISTRY COPYRIGHT 2002 ACS L2

45 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-IN biphenyl]-4-yl- (9CI) C33 H42 N4 O4

MF

Ph
$$CH_2 - C - NH_2 O \\ N - C - CH_2 - N - C - CH_2 - NH - CH_2 - CH_2$$
O (CH₂) 5 - Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl-4-fluoro- (9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

0.76 0.97

STN INTERNATIONAL LOGOFF AT 14:04:27 ON 15 MAY 2002

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SINCE FILE TOTAL

FULL ESTIMATED COST

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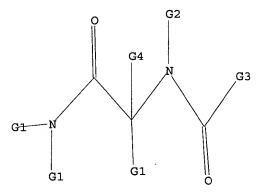
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Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 09852965.str

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb,Ak

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam SAMPLE SEARCH INITIATED 13:03:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 41378 TO ITERATE

2.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

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PROJECTED ITERATIONS:

815485 TO 839635

PROJECTED ANSWERS:

37850 TO 43250

49 ANSWERS

L2

49 SEA SSS SAM L1

=> d scan

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6-methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C28 H33 N5 O4

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):48

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl, [S-(R*,R*)]- (9CI)

MF C34 H58 N4 O7

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(2-fluorobenzoyl)amino]-3,4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl)- (9CI)
- MF C33 H32 F N5 O4

$$\begin{array}{c|c} & & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN .beta.-Alanine, N-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]ph
 enyl]acetyl]-N-(3-phenylpropyl)glycyl-N-(3-phenylpropyl)- (9CI)
- MF C40 H46 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
 methyl ester (9CI)

MF C42 H34 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C37 H37 Cl N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-Nmethylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanylN-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N,N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]- (9CI)

SQL 11

MF C79 H125 N11 O17

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-D-isoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL 10

MF C49 H85 N15 O15

PAGE 1-A ÒН R Me HŅ HN Εt Me HN. HN И Н Мe NH₂ NΗ H_2N (CH₂) 3 Мe ЙH NH2

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-valyl]-L-isoleucyl]-L-asparaginyl]-L-.alpha.-aspartyl]- (9CI)

SQL 5

MF C35 H54 N6 O12

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2 (1H) -Isoquinolinepropanamide, N-(2-amino-2-oxoethyl) -7-[(2,6-difluorobenzoyl) amino] -3,4-dihydro-1-oxo-N-(phenylmethyl) -3-(2-quinolinyl) - (9CI)

MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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SQL 5

MF C38 H61 N5 O11 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L.alpha.-aspartyl]-, mono(trifluoroacetate) (9CI)

SQL 4

MF C20 H31 N5 O7 . C2 H F3 O2

CM 1

Absolute stereochemistry.

$$(CH_2)_{4}$$

$$Me$$

$$O$$

$$O$$

$$N$$

$$S$$

$$CO_2H$$

$$CO$$

CM 2

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)
MF C35 H42 N6 O4

$$\begin{array}{c} O \\ \parallel \\ O \\ CH_2-C-NH_2 \\ \parallel \\ C-N-(CH_2)_3-NEt_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl]- (9CI)

MF C38 H40 N4 O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . C1 H

● HCl

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4-dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)
MF C29 H34 N4 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl[(3-methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
 methyl ester (9CI)
MF C44 H55 Cl N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-1-oxo-Npropyl-3-(2-quinolinyl)-7-[(2,3,5,6-tetrafluoro-4-methylbenzoyl)amino](9CI)

MF C34 H31 F4 N5 O4

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IN D-Phenylalanine, N-[(2E)-5-amino-5-methyl-1-oxo-2-hexenyl]-3-[1,1'-biphenyl]-4-yl-N-methyl-D-alanyl-N-methyl-, trimethylhydrazide (9CI)
MF C36 H47 N5 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Dermorphin, 2-D-arginine-4-(N-methylglycine)- (9CI)

SQL 7

MF C44 H59 N11 O10

PAGE 1-B

__OH

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

PAGE 2-B

PAGE 3-A

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IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

PAGE 2-A

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D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]-IN D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

C37 H51 Cl N4 O7 MF

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[[(3-carboxyphenyl)amino]carbonyl]glycyl-N-methyl-N-phenyl-IN N2-8-quinolinyl- (9CI)

C28 H25 N5 O5 MF

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2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-IN [(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo- (9CI) C33 H33 F2 N5 O5 MF

CH2-CH2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-IN biphenyl]-4-yl- (9CI)

C33 H42 N4 O4 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl4-fluoro- (9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[(2chlorophenyl)methyl]amino]carbonyl]-3,4-dihydro-3-[4-(methylthio)phenyl]-1oxo-N-(3-pyridinylmethyl)- (9CI)

MF C35 H34 Cl N5 O4 S

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & & \\ & & & \\ H_2N-C-CH_2 & & & \\ & & & \\ N & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 7-Oxa-2,5,10,13-tetraazatetradecan-14-oic acid, 10-[2-[[1-(cyclohexylmethyl)-2-hydroxy-5-methylhexyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-2,5-dimethyl-1-(4-morpholinyl)-1,6,9-trioxo-8-(phenylmethyl)-, phenylmethyl ester, [1S-[1R*[R*(R*)],2R*]]-(9CI)

MF C49 H72 N8 O9

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IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)

MF C37 H39 N5 O5 S

PAGE 1-A

O
CH₂-C-NH₂

O
CH₂-C-NH₂

MeO-CH₂-CH₂-C-NH
O

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-D phenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysyl L-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl (9CI)

SQL 13

MF C94 H135 Cl N30 O18

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(2-methoxyphenyl)-1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

MF C37 H36 F3 N5 O5

PAGE 1-A

$$\begin{array}{c} \text{CF}_{3} \\ \text{CH}_{2} \\ \text{NH} \\ \text{C} \\ \text{C}_{1} \\ \text{C}_{2} \\ \text{C}_{1} \\ \text{C}_{2} \\ \text{C}_{2} \\ \text{C}_{3} \\ \text{C}_{1} \\ \text{C}_{2} \\ \text{C}_{2} \\ \text{C}_{3} \\ \text{C}_{2} \\ \text{C}_{3} \\ \text{C}_{2} \\ \text{C}_{3} \\ \text{C}_{4} \\ \text{C}_{2} \\ \text{C}_{4} \\ \text{C}_{4} \\ \text{C}_{5} \\ \text{C}_{5}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Alaninamide, N-[(tetrahydro-2-furanyl)carbonyl]glycyl-3-(2-naphthalenyl)D-alanyl-4-chloro-D-phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-N-methylL-tyrosyl-N6-(3-pyridinylcarbonyl)-L-lysyl-L-leucyl-N6-(1-methylethyl)-Llysyl-L-prolyl-, (S)- (9CI)

SQL 11

MF C85 H111 Cl N16 O16

CI COM

PAGE 1-B

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L2    49 ANSWERS    REGISTRY    COPYRIGHT 2002 ACS
IN    4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (phenylmethyl) amino] carbonyl] phenyl] methyl] -1,2,3,4-tetrahydro-3-(4-hydroxyphenyl) -1-oxo-N-[[4-(trifluoromethyl) phenyl] methyl] - (9CI)
MF    C41 H35 F3 N4 O5
```

$$\begin{array}{c} CF_3 \\ CH_2 \\ NH \\ NH \\ C = 0 \\ CH_2 - N \\ CH_2$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Ornithinamide, L-leucyl-N2-methyl-N-2-naphthalenyl-, trifluoroacetate (9CI)

MF C22 H32 N4 O2 . x C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Glycinamide, N-[[(3-methylphenyl)amino]carbonyl]glycyl-N-methyl-N2-[3-[2oxo-2-(phenylamino)ethoxy]phenyl]-N-phenyl- (9CI)

MF C33 H33 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl
ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[[2-(trimethylsilyl)ethoxy]carbonyl]amino]-D-alanyl-L-alanyl-S-[(acetylamino)methyl]-N-methyl-L-cysteinyl-N-methyl-L-valyl-(2R)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-.beta.-alanyl-L-alanyl-S-[(acetylamino)methyl]-N-methyl-L-cysteinyl-N-methyl-, methyl ester (9CI)
SQL 8

MF C55 H100 N12 O17 S2 Si

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide
, 45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)

MF C88 H115 N33 O32

PAGE 1-A

Me NH

$$CH_2$$
 $C = 0$
 $N - CH_2 - C - NH_2$
 CH_2
 CH_2

PAGE 1-B

PAGE 1-C

PAGE 2-C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-N-methyl-3-(2-naphthalenyl)-D-alanyl-N, N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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SQL 5

MF C41 H63 N5 O8 S

PAGE 1-A

PAGE 1-B

— CH₂− SMe

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE ENTRY TOTAL SESSION

0.76

0.97

09/852,965

STN INTERNATIONAL LOGOFF AT 13:04:40 ON 15 MAY 2002

L4 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 1970:477105 CAPLUS

DN 73:77105

TI Preparation and properties of mesoionic oxazolones

AU Bayer, Horst O.; Huisgen, Rolf; Knorr, Rudolf; Schaefer, Fred C.

CS Inst. Org. Chem., Univ. Muenchen, Munich, Ger.

SO Chem. Ber. (1970), 103(8), 2581-97 CODEN: CHBEAM

DT Journal

LA German

IT 28544-59-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 28544-59-4 CAPLUS

CN Benzamide, N-methyl-N-[.alpha.-(p-tolylcarbamoyl)benzyl]- (8CI) (CA INDEX NAME)

L4 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 1967:2461 CAPLUS

DN 66:2461

TI 2,3,4,5-Tetrahydro-1H-3-benzazepin-1-ones and hexahydroimidazoisoquinolines

AU Hazebroucq, Georges

CS Pharm., Centrale Hop., Paris, Fr.

SO Ann. Chim. (Paris) (1966), 1(5/6), 221-54 CODEN: ANCPAC

DT Journal

LA French

IT 14174-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 14174-20-0 CAPLUS

CN Acetanilide, 2-[N-(3,4-dimethoxyphenethyl)benzamido]-2-phenyl- (8CI) (CA INDEX NAME)